Forum for Electromagnetic Research Methods and Applications Technologies (FERMAT)

Parallel Computational Approach to Gradient Based EM Optimization of Microwave Structures

By

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Abstract: Electromagnetic (EM) based optimization and design closure is an essential part of RF and microwave design cycle. The main objective of this thesis is to develop a new gradient based EM optimization technique which exploits parallel computations. The proposed EM optimization technique achieves speed up in the optimization process even if a coarse model is not available. Speed up in optimization has been achieved by using large and effective optimization updates in each iteration which resulted in fewer optimization iterations. The first contribution of the thesis is the development of a trust-region based optimization technique which uses parallel computational approach. In the proposed method, we deliberately increase the number of fine model evaluations without increasing the computation time by using a parallel computational approach. A large number of fine model evaluations allows us to build a surrogate model valid in a large neighborhood. These valid surrogate models are used to achieve large and effective optimization updates. The second major contribution of the thesis is the EM optimization decomposition approach to address the challenges in EM optimization with many design variables. This proposed method decomposes a single large EM optimization problem into multiple smaller sub-optimizations to improve the optimization efficiency. Multiple sub-optimizations are formulated to be independent so that the parallel computations can be exploited to evaluate concurrent sub-optimization updates. The resultant vector, a combined vector of sub-optimization updates, will be closer to the optimal solution. Furthermore, the optimization update of the proposed approach is much larger in comparison with the optimization update without decomposition.

Keywords: Decomposition, electromagnetic (EM) optimization, gradient optimization, microwave filter, parallel, sub-optimization, surrogate model, trust region.

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Parallel Computational Approach to Gradient based EM Optimization of Microwave Structures

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Carleton UNIVERSITY | Faculty of Engineering and Design

Outline

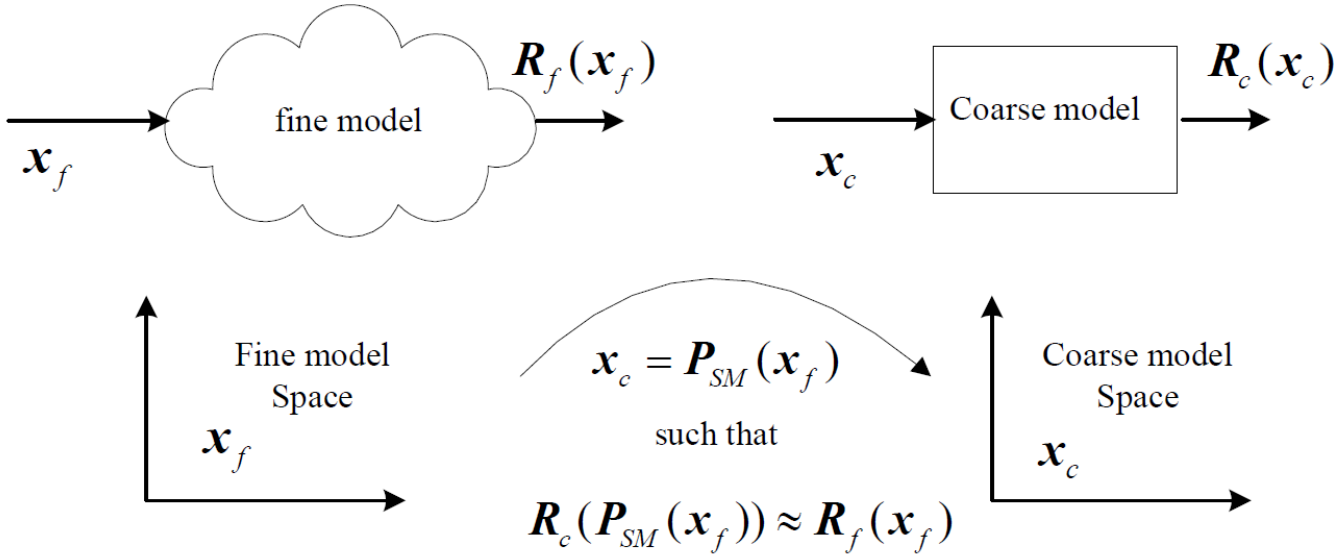
- Introduction
- Existing Techniques
- Proposed Optimization –I
- Proposed Optimization –II
- Future Directions

Motivation

- EM based simulation and optimization - more important for microwave design.
- Repetitive changes to geometrical parameters such as length & width to find the optimal design parameters.
- Huge computational cost and large CPU time.
- EM complexity, stringent design specifications and shorter design cycle – faster, accurate and automated.

Existing Techniques

- Direct EM optimization
- Space mapping – surrogate based optimization technique
  - Fewer fine model evaluations
  - Exploits coarse models (empirical or equivalent circuits)

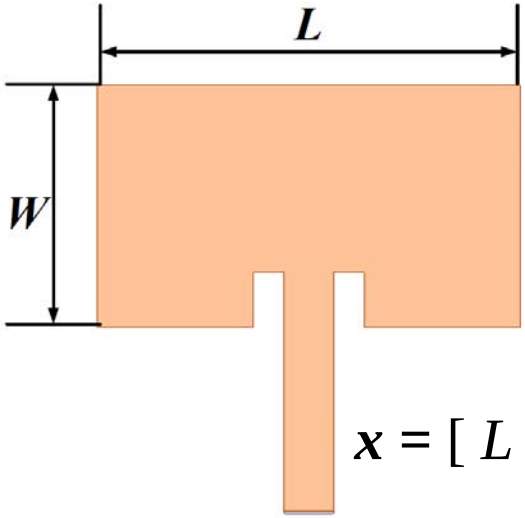


- Coarse and fine mesh space mapping – no equivalent circuits

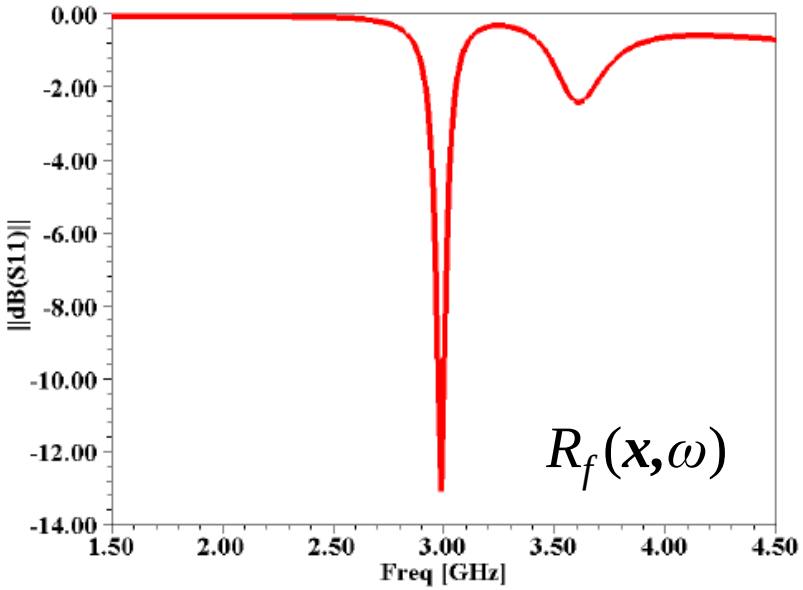
Objective

- Speed up EM optimization.
- Exploit parallel computation power
- Large CPU time for EM optimization- needs to addressed
- Our goal is to formulate a methodology that
  - exploits parallel computation,
  - uses gradient based optimization method (faster)
  - and achieve speed up in the optimization technique.
  - Applicable when no coarse models are available.

Optimization Problem Definition



$\boldsymbol{x} = [\ L \quad W\ ]^{\mathrm{T}}$



- Original optimization problem

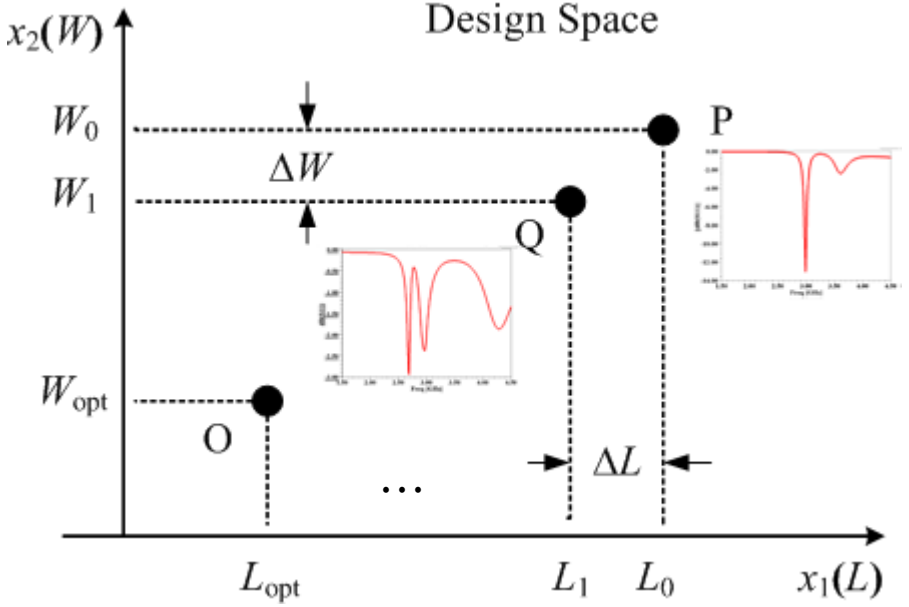
$$\boldsymbol{x}^* = \arg\min_{x \in X} U\left(R_f(\boldsymbol{x},\omega)\right)$$

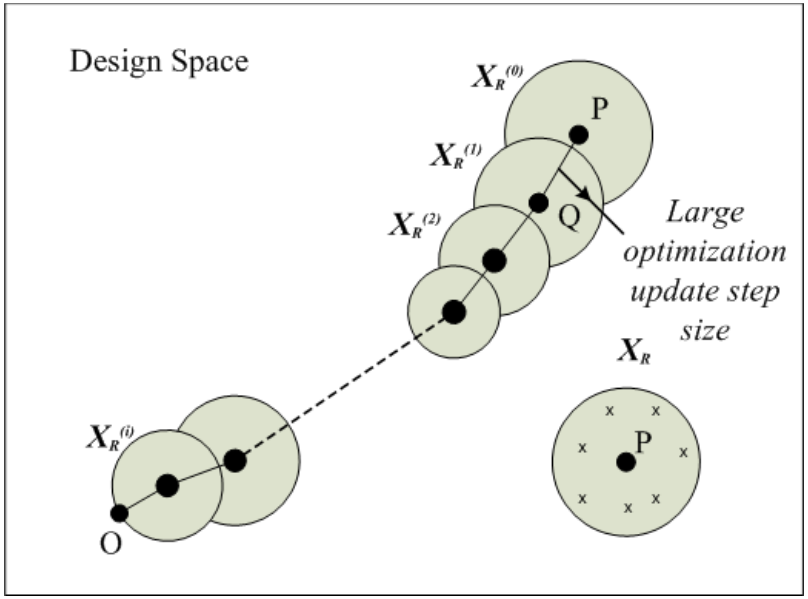
Where $\boldsymbol{x}$ denotes the design vector containing geometrical design variables

$R_f(\boldsymbol{x},\omega)$ denotes the response of the fine model, and

U represents the objective function.

Concept





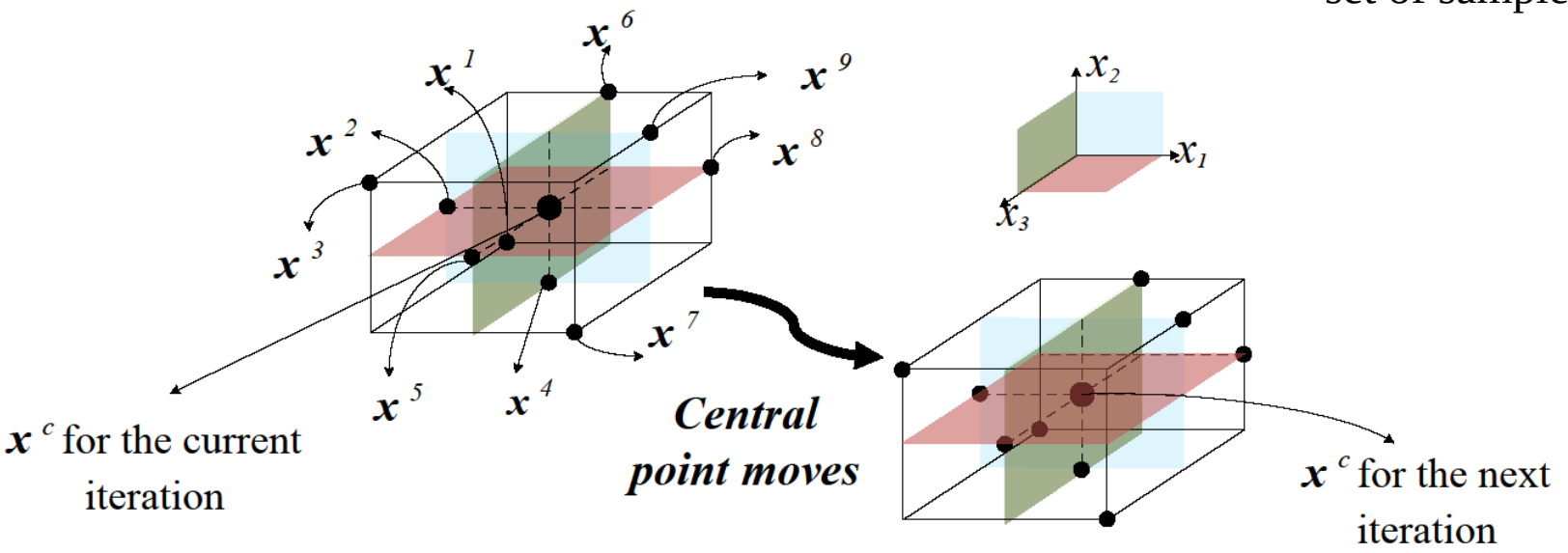
Large region or small region ??

Guaranteed Convergence ??

Orthogonal Array Sampling in the Trust Region for 3 Design Variables

Design variables : $\boldsymbol{x} = [\, x_1\ x_2 \ldots x_n]^{\mathrm{T}}$

$\left\{ \boldsymbol{x}^1, \boldsymbol{x}^2, \cdots, \boldsymbol{x}^9 \right\}$
- set of sampled points



$\boldsymbol{x}^c = \left[x_1^c\ \ x_2^c\ \cdots\ x_n^c \right]^T$ **Central point** in the current iteration.

$\boldsymbol{X}_R$ - **Trust Region**

$$\boldsymbol{X}_R = \left\{ \boldsymbol{x} \;\middle\|\; x_j^c - \delta_j \le x_j \le x_j^c + \delta_j ; \text{ where } j = 1, 2, \cdots, n \right\}$$

Parallel Computation

- Implemented on hybrid distributed-shared memory architecture.
  - Distribute the data samples.
  - Perform fine model evaluations such that each processor performs one EM simulation (one fine model evaluation).

$$\left\{ R_f(\boldsymbol{x}^m, \omega) \,|\, m = 1, 2, \cdots, N_s \right\}$$

Speed up

$$S_p = \frac{T_s + (\sum_{m=1}^{N_s} T_m + T_p) i_{total}}{T_s + \left(\frac{N_s}{P} \max_{1 \le m \le N_s} \{T_m\} + T_p + T_{ov} \right) i_{total}}$$

Parallel efficiency

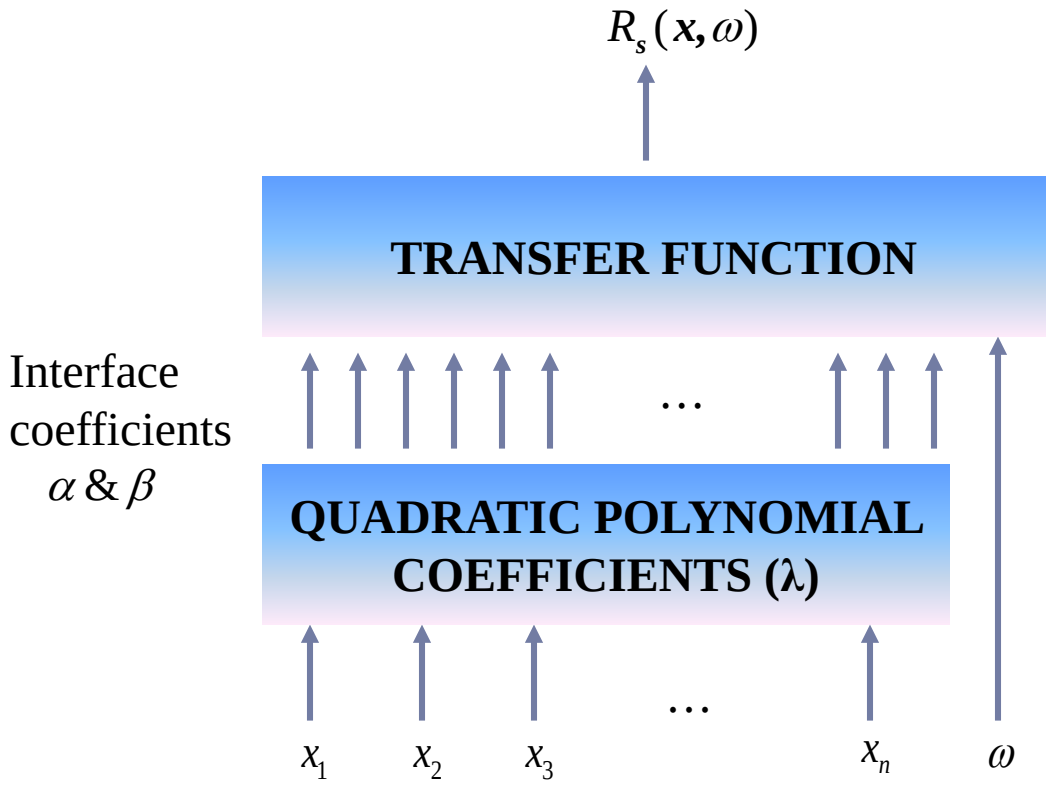
$$\eta = \frac{S_p}{P}$$

- Max Parallel efficiency - minimizing overhead CPU time and surrogate model generation and optimization CPU time per iteration

Surrogate Modeling using Multiple Points

- Transfer functions are used for constructing the surrogate.

- The surrogate model response $R_s(\boldsymbol{x}^m, s)$



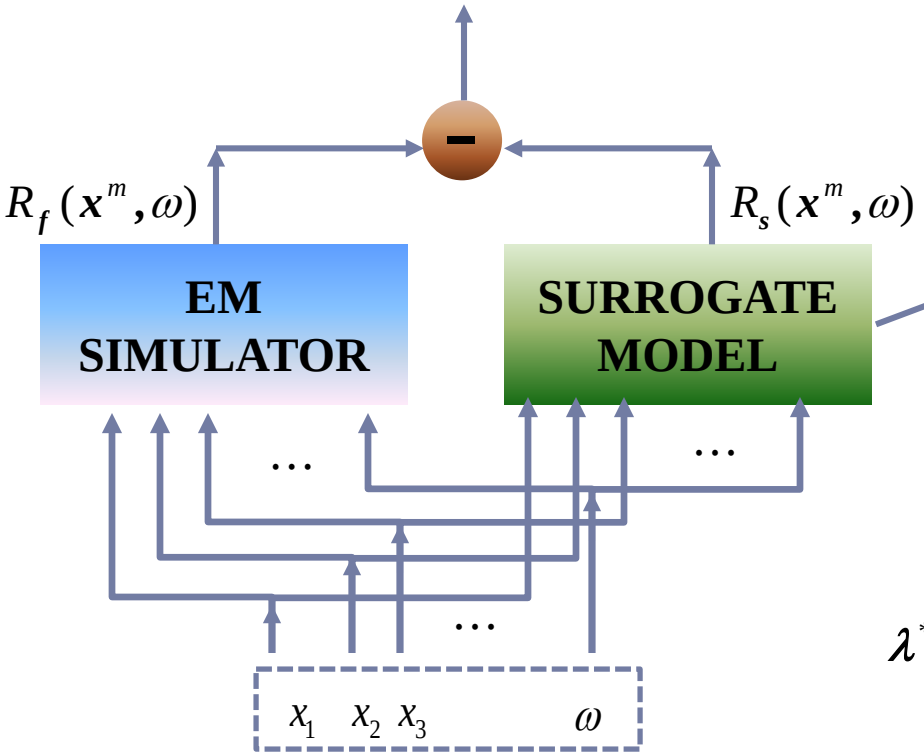
$$R_s(\boldsymbol{x}^m, \hat{z}) = \frac{\sum_{l=0}^{M} \alpha_l^m \hat{z}^l}{1 + \sum_{k=1}^{N} \beta_k^m \hat{z}^k}$$

$$\alpha_r^m = g_r(\boldsymbol{\lambda}_r, \boldsymbol{x}^m)$$

Finding Weighting Vectors

- The new weighting vectors

$$E(\lambda,\omega) = \left\| R_s(\boldsymbol{x}^m,\omega) - R_f(\boldsymbol{x}^m,\omega) \right\|$$



Optimize weighting vectors

$$\lambda^* = \arg\min_{\lambda} \left(\sum_{\omega\in\Omega} \sum_{m=1}^{N_s} E(\lambda,\omega) \right)$$

Optimization Update and Trust Radius Update

- Surrogate model optimization update $\boldsymbol{x}^{new} = \arg\min_{\boldsymbol{x} \in X_R} U\left(R_s(\boldsymbol{x}, \omega)\right)$

Predicted value of Objective Function @ x^{new}	$U\left(R_s(\boldsymbol{x}^{new}, \omega)\right)$
Actual value of Objective Function @ x^{new}	$U\left(R_f(\boldsymbol{x}^{new}, \omega)\right)$
Actual value of Objective Function @ x^c	$U\left(R_f(\boldsymbol{x}^{c}, \omega)\right)$

- Verify, $\boldsymbol{x}^{new}$ is the new prospective update or not,

$$r_a = -1, \ \textit{if} \ U\left(R_f(\boldsymbol{x}^{new}, \omega)\right) > U\left(R_f(\boldsymbol{x}^{c}, \omega)\right)$$

$$= \frac{U\left(R_f(\boldsymbol{x}^{c}, \omega)\right) - U\left(R_f(\boldsymbol{x}^{new}, \omega)\right)}{U\left(R_f(\boldsymbol{x}^{c}, \omega)\right) - U\left(R_s(\boldsymbol{x}^{new}, \omega)\right)}, \ \text{Otherwise}$$

Trust radius update

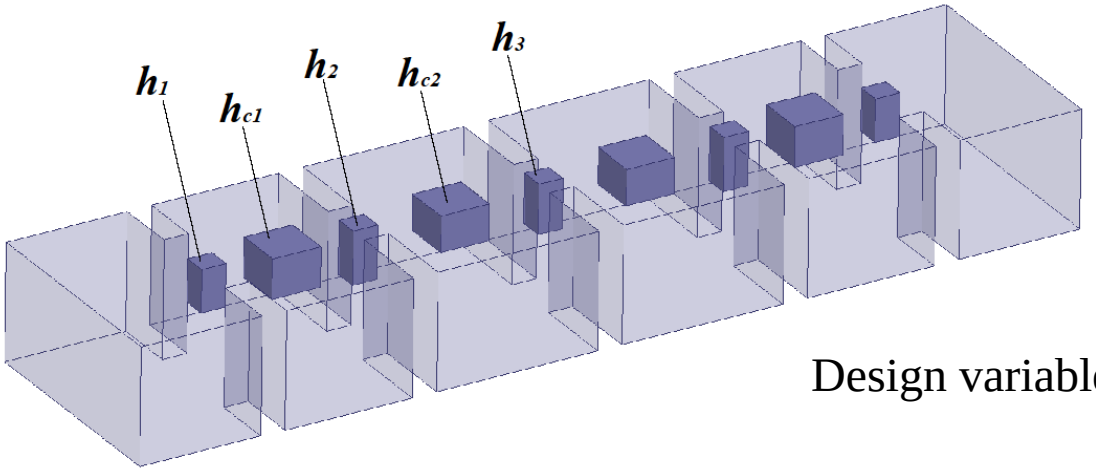
$$\delta^{new} = \begin{cases} c_1\delta, & r_a < 0.1 \\ \min(c_2\delta, \Delta^{\max}), & r_a > 0.75 \\ \delta, & \textit{Otherwise} \end{cases}$$

Termination Conditions

$$\left\| \boldsymbol{x}^{c} - \boldsymbol{x}^{new} \right\| \le \varepsilon$$

$$U\left(R_f(\boldsymbol{x}^{new}, \omega)\right) \le 0$$

Four Pole Waveguide Example



Design variables : $\boldsymbol{x} = [\, h_1\ h_2\ h_3\ h_{c1}\ h_{c2}]^T$

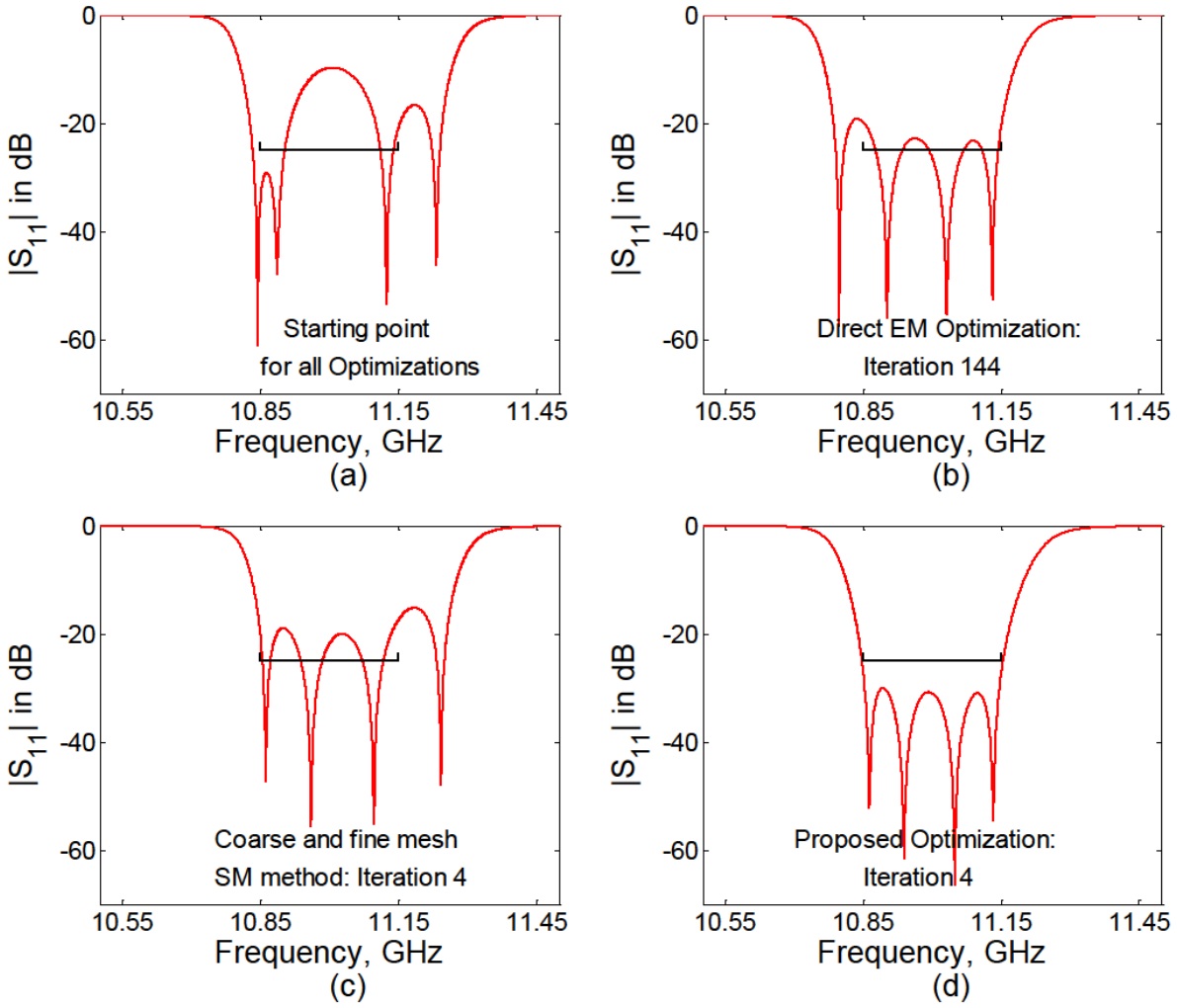
Design Specifications : $\|S_{11}\| \leq -25\text{dB}$ for $10.85\text{GHz} \leq \omega \leq 11.15\text{GHz}$

	Case 1: Good Starting Point	Case 2: Bad Starting Point
Starting point	$\boldsymbol{x}^c = [3.3\ 4.4\ 4.0\ 3.28\ 2.91]^T$	$\boldsymbol{x}^c = [3.0\ 4.1\ 3.5\ 3.3\ 3.0]^T$

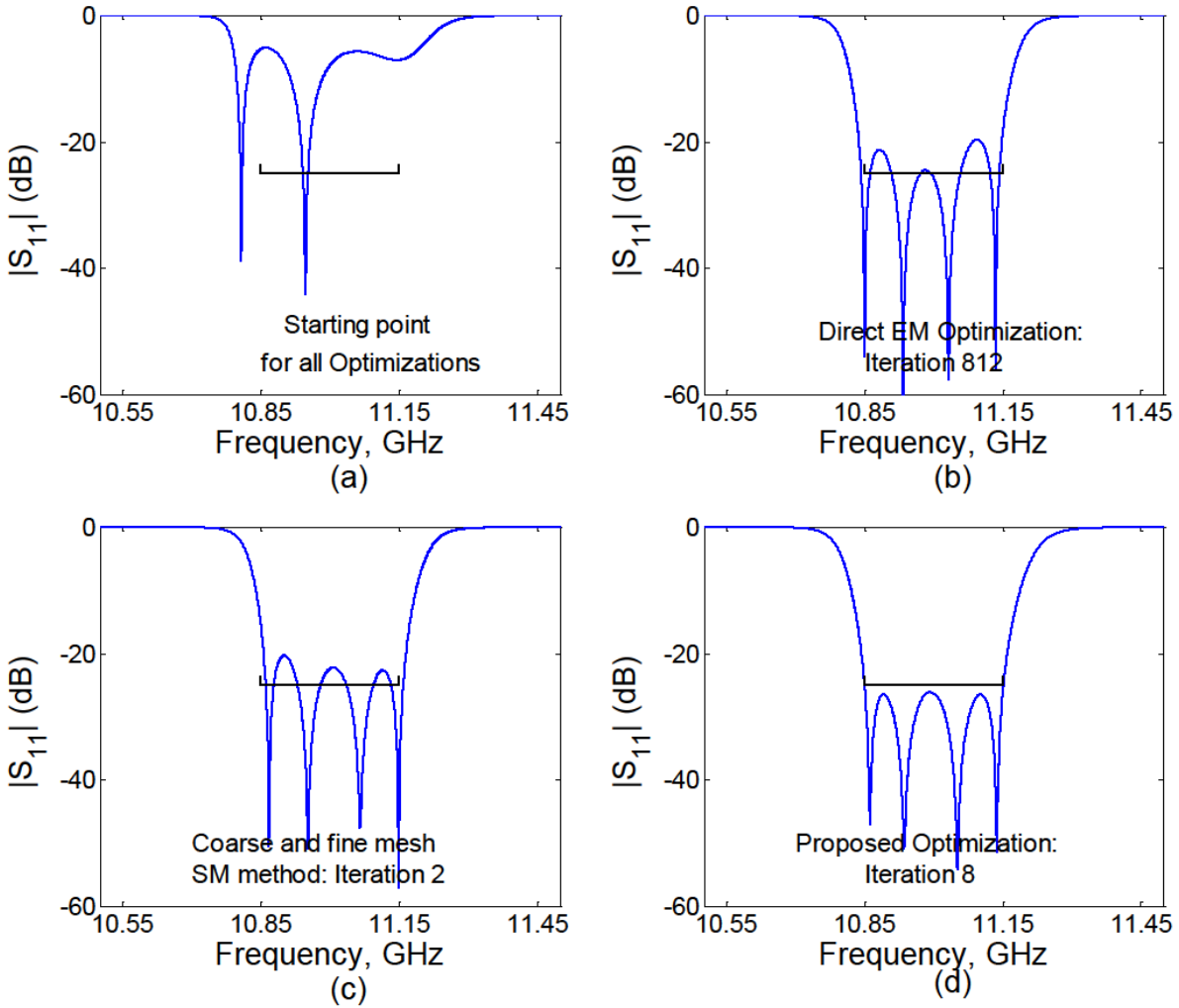
Initial trust radius : $\boldsymbol{\delta} = [0.132\ 0.176\ 0.16\ 0.0656\ 0.0582]^T$ (in mm) which is $[4\ 4\ 4\ 2\ 2]\ ]^T$ %

Maximum trust radius : $\Delta^{max} = [0.132\ 0.176\ 0.16\ 0.0656\ 0.0582]^T$ (in mm)

Comparison of Different Optimization Methods for a Good Starting Point



Comparison of Different Optimization Methods for a Bad Starting Point

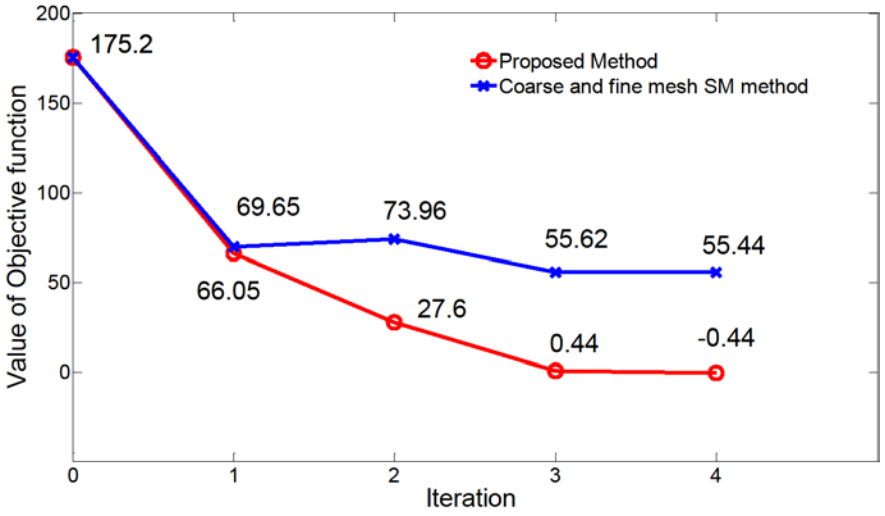


CPU Time Comparison of Different Optimization methods for a Bad Starting Point

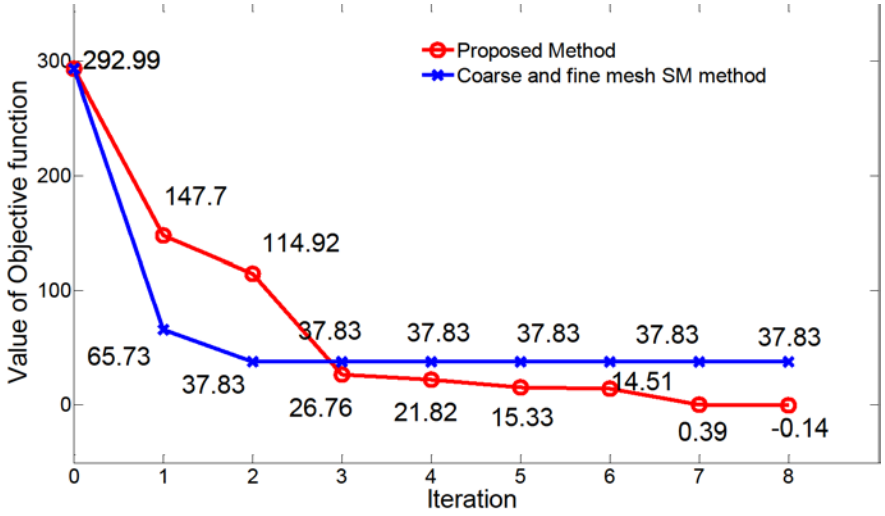
Optimization	Direct EM optimization	Coarse and fine mesh SM optimization	Proposed optimization
Fine model evaluation time per sample	2m 5s	2m 5s	**2m 30s**
No. of fine model evaluations in parallel per iteration	1	1	25
No. of iterations	812	2	8
No. of coarse model evaluations	-	526	-
Time for each coarse model evaluation	-	27s	-
Total time	28h 19m	242.95m	36.86m+2.82m =39.69m

Objective Function Value Comparison

Optimization using a Good Starting point



Optimization using a Bad Starting Point

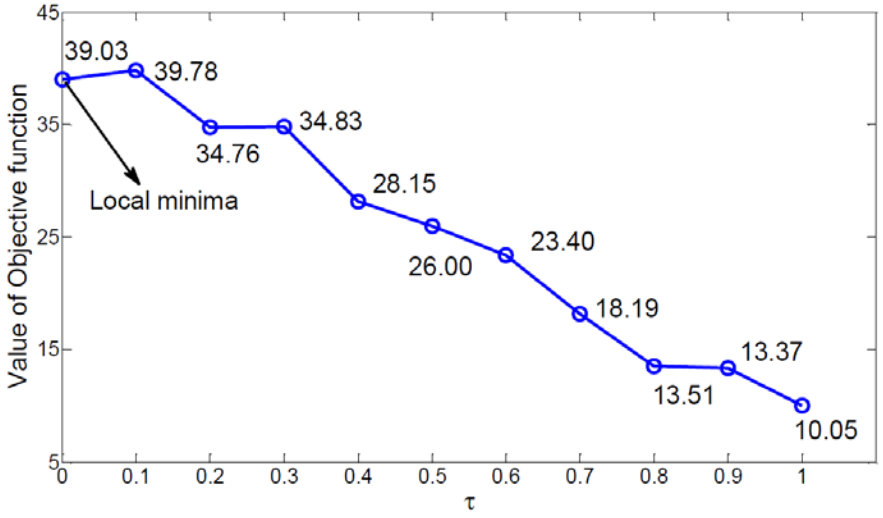


Speed Up Factor **:** 15.69	Speed Up Factor : 16.74
Parallel Efficiency : 62.75%	Parallel Efficiency : 66.9%

Confirming the Solution from Direct EM Optimization is a Local Minima

	Value of objective function	
Solution of direct EM optimization	39.028	
Perturbation	+ve direction	-ve direction
Perturb x_1 of $\boldsymbol{x}^{em}$	43.231	43.950
Perturb x_2 of $\boldsymbol{x}^{em}$	44.821	43.709
Perturb x_3 of $\boldsymbol{x}^{em}$	44.587	44.336
Perturb x_4 of $\boldsymbol{x}^{em}$	49.329	45.609
Perturb x_5 of $\boldsymbol{x}^{em}$	48.220	48.264

$$\boldsymbol{x}^{sample} = \boldsymbol{x}^{em} + \tau(\boldsymbol{x}^{new} - \boldsymbol{x}^{em})$$



The new solution from one iteration of the proposed optimization jumps the local minima solution obtained from direct EM optimization

Contributions-I

- The proposed method achieves speedup even if a coarse model is not available.
- The proposed method deliberately increases the number of fine model evaluations without increasing computational time by using a parallel computation approach.
- Speed up is achieved by using large and effective optimization updates.

Next Challenge (Increase in *n*)

- Major issue - **Scalability** (w.r.t input design variables)
- Volume of search space increases as the order of *n*
- Increased likelihood of getting trapped in local minima using conventional gradient based methods.
- With increase in *n* the number of possible design variations that are needed to predict EM behaviour increases which results in the decreased validity range for the surrogate model.

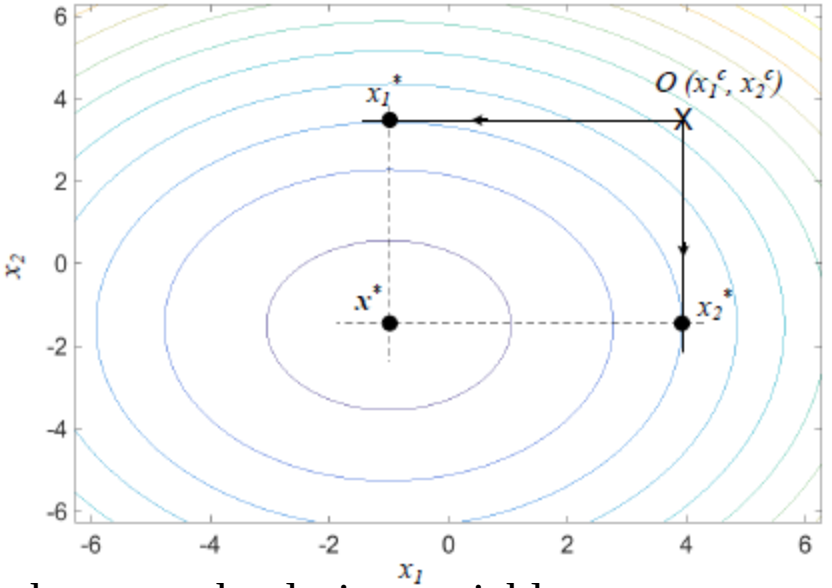
Solution

For illustration, suppose $\boldsymbol{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T$

Taylor series expansion :

$$R_f(\boldsymbol{x}, \omega_0) = B_0 + B_1 x_1 + B_2 x_2 + B_3 x_1^2 + B_4 x_1 x_2 + B_5 x_2^2$$

$$B_4 = \frac{\partial^2 y}{\partial x_1 \partial x_2} \rightarrow \text{Second order derivative}$$



B_4 – **eccentricity or measure of interaction** between the design variables

$B_4 = 0$; x_1 and x_2 are **independent and separable**.

Decomposition of original optimization problem into two smaller sub-opts

$$x_1^* = \arg \min_{x_1 \in \tilde{X}^{(1)}} U\left(\tilde{R}_f(x_1, \omega_0)\right) \qquad x_2^* = \arg \min_{x_2 \in \tilde{X}^{(2)}} U\left(\tilde{R}_f(x_2, \omega_0)\right)$$

Optimal Solution $\rightarrow$ $\boldsymbol{x}^* = \begin{bmatrix} x_1^* & x_2^* \end{bmatrix}^T$

Decomposition

The decomposition method is sub-divided as

- Measure of interactions (eccentricity) for all design variables (i.e., second order derivatives)
- Iteratively identify strongly interacting design variables.
- Form the sub-design vectors for further sub-optimization

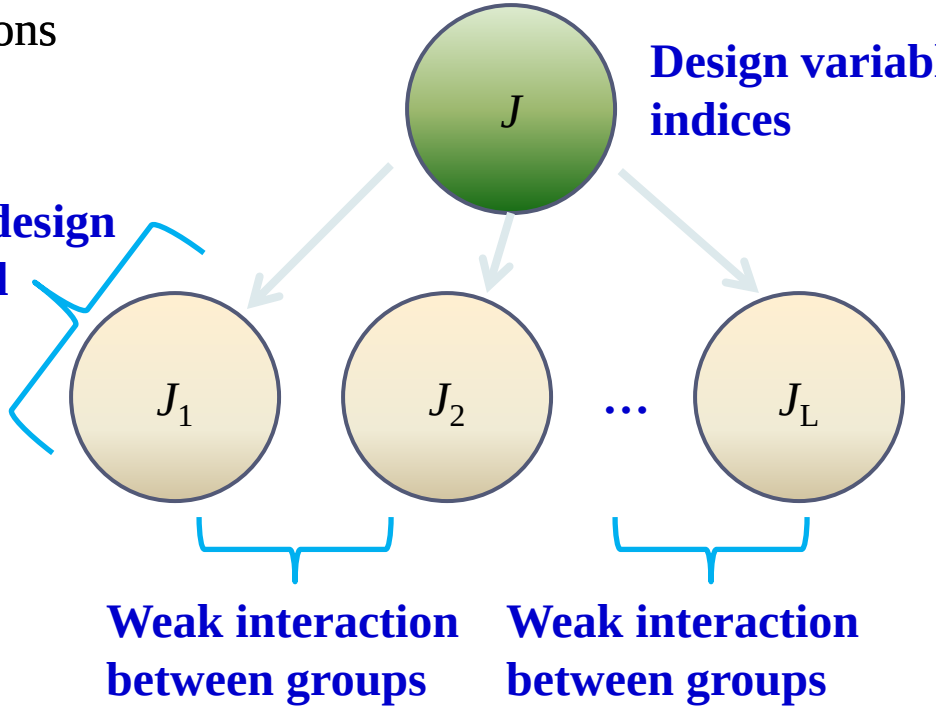
Measure of interaction

$$\boldsymbol{C} = \begin{pmatrix} C_{11} & \cdots & C_{1n} \\ \vdots & \ddots & \vdots \\ C_{n1} & \cdots & C_{nn} \end{pmatrix}_{n \times n}$$

$$C_{ab} = \sum_{q=1}^{N_f} \left\| \frac{\partial S_{q,a}}{\partial x_b} \right\| = \sum_{q=1}^{N_f} \left\| \frac{\partial^2 R_f(\boldsymbol{x}, \omega_q)}{\partial x_a \partial x_b} \right\|$$

Identification of strongly Interacting Design Variables

L - number of groups or sub-optimizations



Strongest interaction

$$C_{kl} = \left\{ \max_{\substack{1<a\le n \\ a<b\le n}} C_{ab},\ a \notin J_i \vee b \notin J_i \right.$$

Form the i^{th} sub design vector

J – represents the index set of sub design vector

$$J_i = \begin{cases} J_i \cup \{k\} \cup \{l\},\ if\ k \notin J_i \wedge l \notin J_i \wedge (d_i < d_{\min}) \\ J_i \cup \{k\},\ if\ k \notin J_i \wedge l \in J_i \wedge (d_i < d_{\min}) \\ J_i \cup \{l\},\ if\ k \in J_i \wedge l \notin J_i \wedge (d_i < d_{\min}) \end{cases}$$

Flow Chart with Example

$$C = \begin{pmatrix} - & 101 & 134 & 207 & 15 & 21 & 13 & 7 & 5 & 76 & 7 \\ - & - & 271 & 407 & 21 & 46 & 43 & 37 & 20 & 120 & 15 \\ - & - & - & 1721 & 53 & 54 & 48 & 40 & 30 & 206 & 35 \\ - & - & - & - & 9 & 13 & 17 & 23 & 14 & 53 & 12 \\ - & - & - & - & - & 116 & 78 & 26 & 19 & 286 & 28 \\ - & - & - & - & - & - & 1 & 1 & 1 & 4 & 1 \\ - & - & - & - & - & - & - & 2 & 1 & 11 & 2 \\ - & - & - & - & - & - & - & - & 3 & 12 & 3 \\ - & - & - & - & - & - & - & - & - & 38 & 6 \\ - & - & - & - & - & - & - & - & - & - & 12 \\ - & - & - & - & - & - & - & - & - & - & - \end{pmatrix}$$

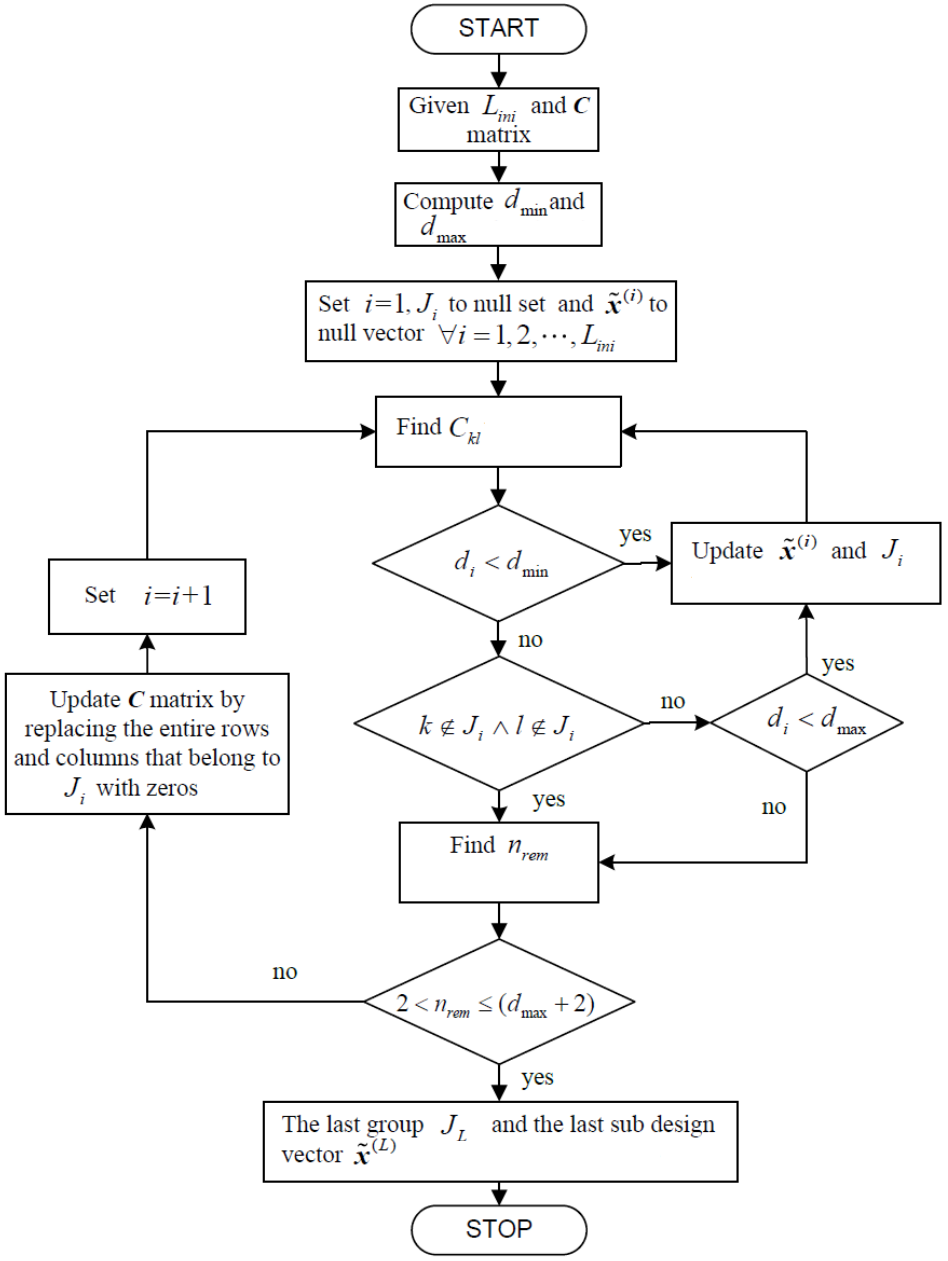
$n = 11,\ L_{ini} = 3,\ d_{min} = 3,\ d_{max} = 5$

$J_1 = \{3, 4, 2\}$

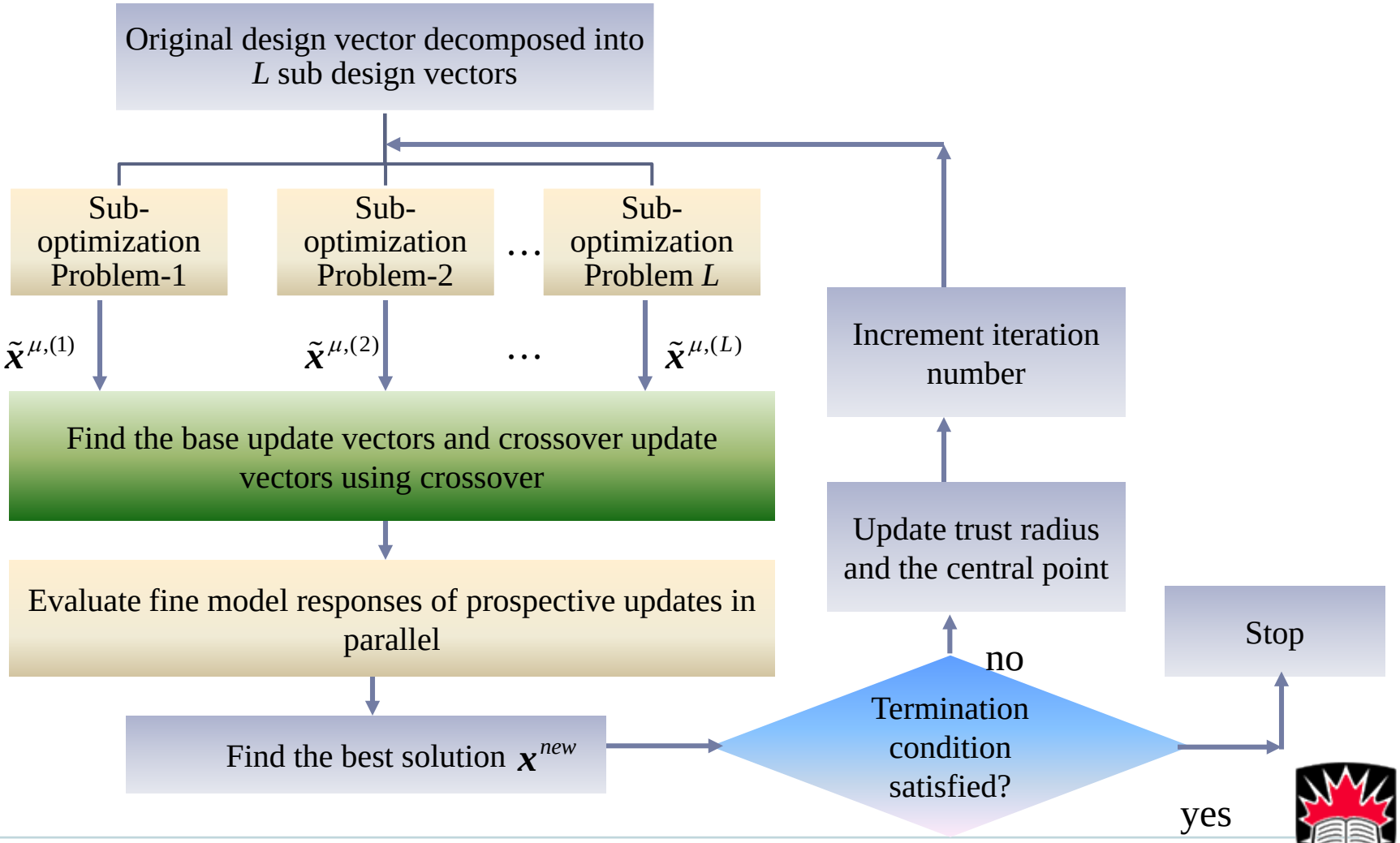
$J_2 = \{5, 10, 6, 7, 1\}$

$J_3 = \{8, 9, 11\}$

Index sets for the sub design vectors



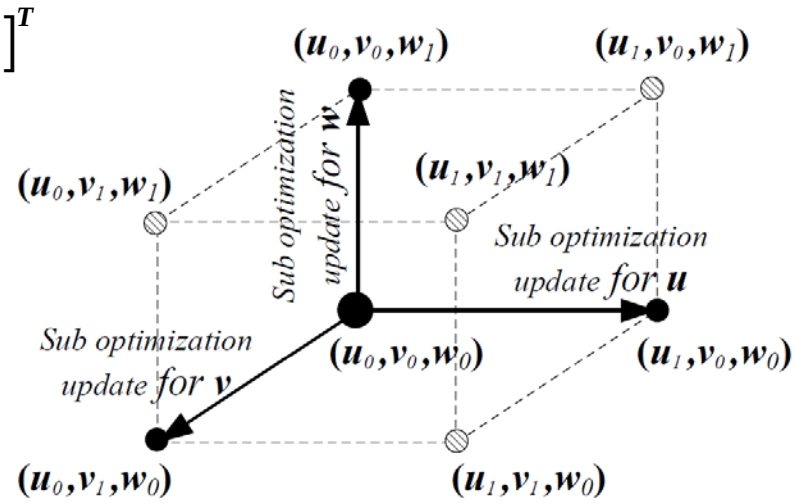
Parallel Formulation for Sub-optimizations

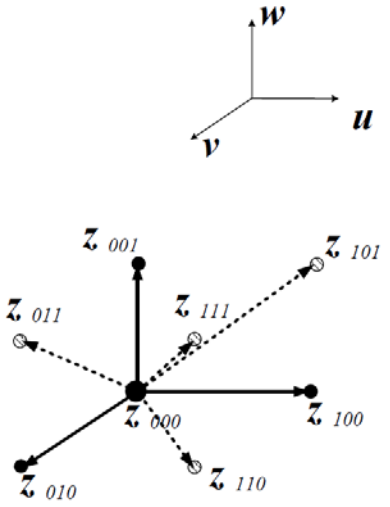


Crossover

- Combining the sub-optimization solution of one subspace with the sub-optimization solutions of one or more subspaces.
- Allows us to directly jump to new optimization update without iteratively searching for the optimal solution in redundant search spaces.
- Span the entire optimization space effectively and efficiently.

$$z = [u\ v\ w]^T$$





Optimization Update after Crossover using a Three Variable Example

Central point in current iteration

Base update vector

Crossover update vector

$$\boldsymbol{z}_{000} = \begin{bmatrix} \tilde{\boldsymbol{x}}^{c,(1)} \\ \tilde{\boldsymbol{x}}^{c,(2)} \\ \tilde{\boldsymbol{x}}^{c,(3)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_0 \\ \boldsymbol{v}_0 \\ \boldsymbol{w}_0 \end{bmatrix} \qquad \boldsymbol{z}_{100} = \begin{bmatrix} \tilde{\boldsymbol{x}}^{\mu,(1)} \\ \tilde{\boldsymbol{x}}^{c,(2)} \\ \tilde{\boldsymbol{x}}^{c,(3)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{v}_0 \\ \boldsymbol{w}_0 \end{bmatrix} \qquad \boldsymbol{z}_{110} = \begin{bmatrix} \tilde{\boldsymbol{x}}^{\mu,(1)} \\ \tilde{\boldsymbol{x}}^{\mu,(2)} \\ \tilde{\boldsymbol{x}}^{c,(3)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_1 \\ \boldsymbol{v}_1 \\ \boldsymbol{w}_0 \end{bmatrix}$$

The best solution is calculated as

$$\boldsymbol{z}^{new} = \arg\min_{\boldsymbol{z}\in\boldsymbol{Z}} U\left(R_f(\boldsymbol{z},\omega)\right) \qquad \text{where,} \qquad \boldsymbol{Z} = \left\{\boldsymbol{z}_{100}, \boldsymbol{z}_{010}, \boldsymbol{z}_{001}, \boldsymbol{z}_{110}, \boldsymbol{z}_{101}, \boldsymbol{z}_{011}, \boldsymbol{z}_{111}\right\}$$

Optimization update

$$\boldsymbol{x}^{new} = \boldsymbol{z}^{new}$$

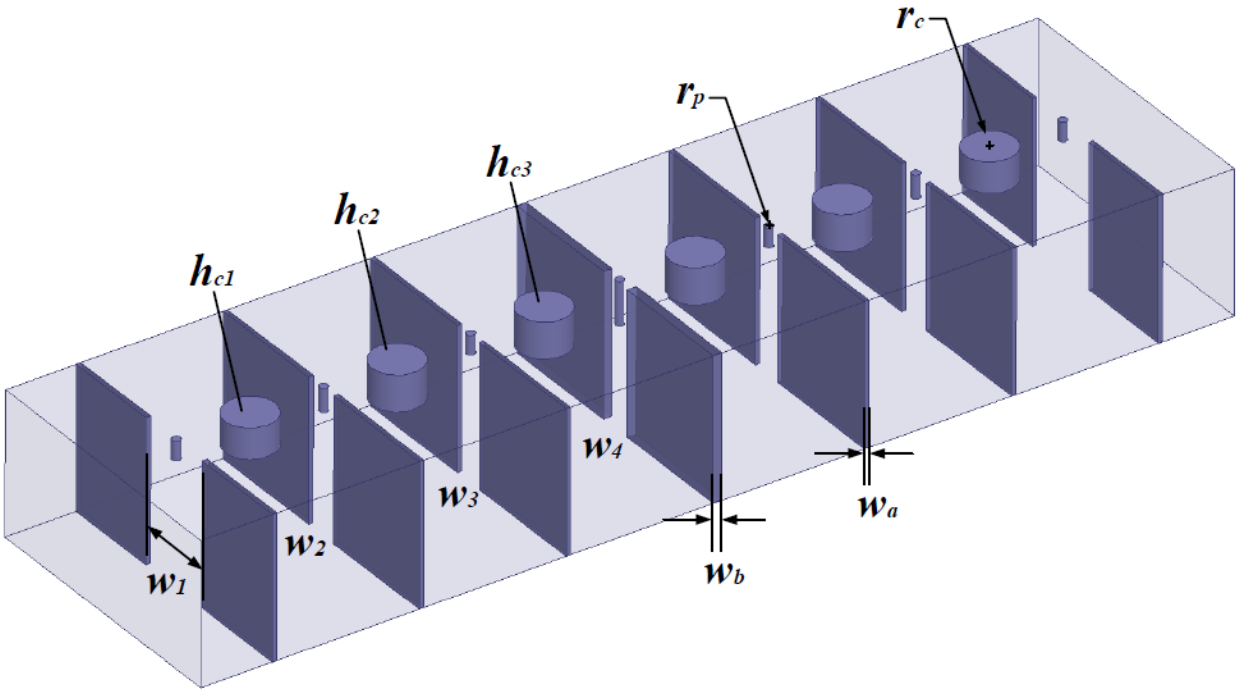
Trust radius update

$$\delta^{new,(i)} = \begin{cases} \delta^{\mu,(i)}, \; if \;\; \boldsymbol{x}^{\mu,(i)} \subset \boldsymbol{z}^{new} \\ \delta^{(i)}, \; if \;\; \boldsymbol{x}^{\mu,(i)} \not\subset \boldsymbol{z}^{new} \end{cases}$$

Termination Conditions

$$\left\|\boldsymbol{x}^{c} - \boldsymbol{x}^{new}\right\| \le \varepsilon \qquad \text{or} \qquad U\left(R_f(\boldsymbol{x}^{new},\omega)\right) \le 0$$

Example-2



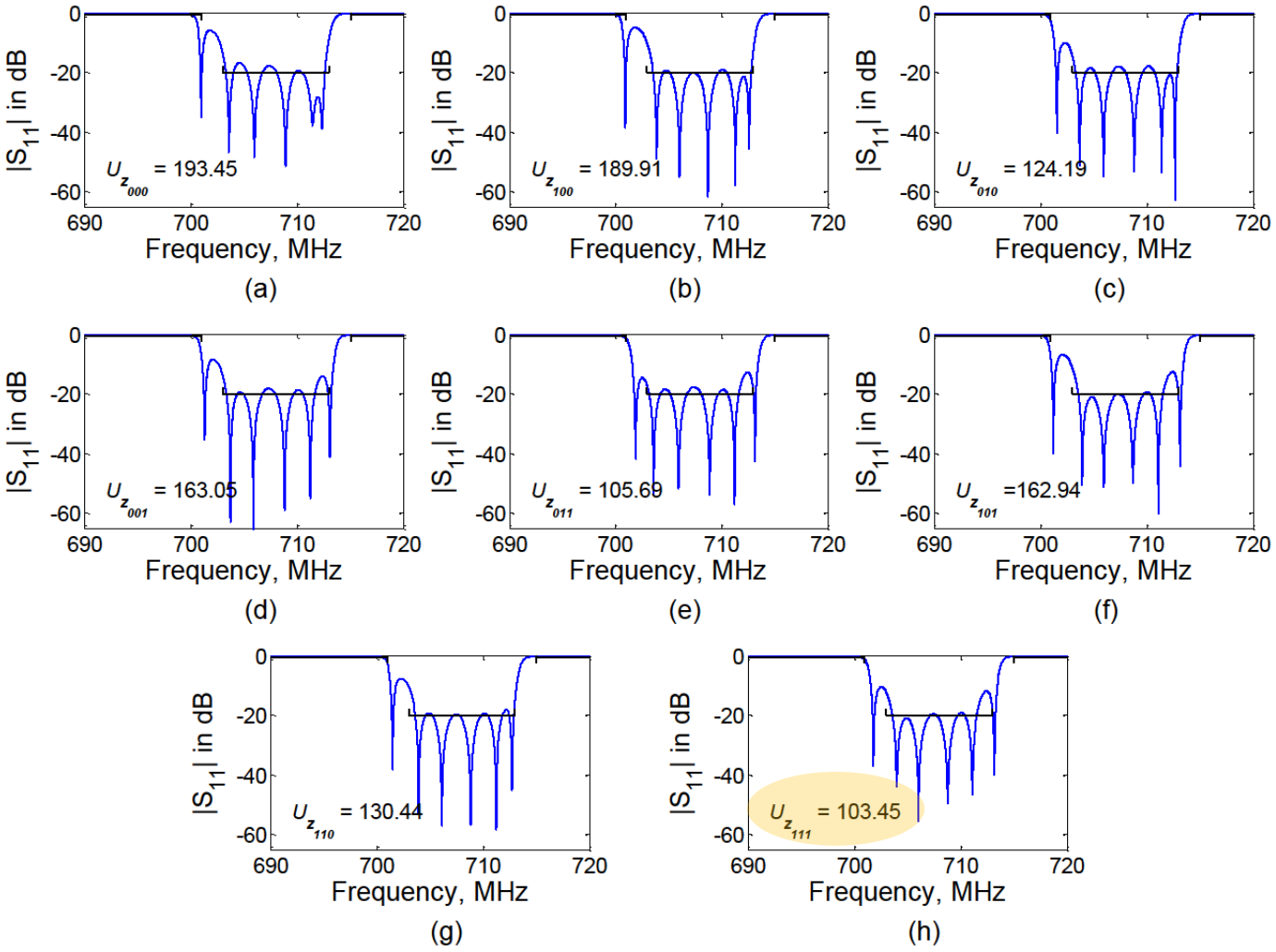
Design variables : $\boldsymbol{x} = [\, h_{c1}\ h_{c2}\ h_{c3}\ r_c\ r_p\ w_1\ w_2\ w_3\ w_4\ w_a\ w_b]^T$

Design Specifications : $||S_{11}|| \leq$ -20dB for 703 MHz $\leq \omega \leq$ 713 MHz and
$||S_{21}|| \leq$ -15dB for 690 MHz $\leq \omega \leq$ 701 MHz and
$||S_{21}|| \leq$ -15dB for 715 MHz $\leq \omega \leq$ 720 MHz

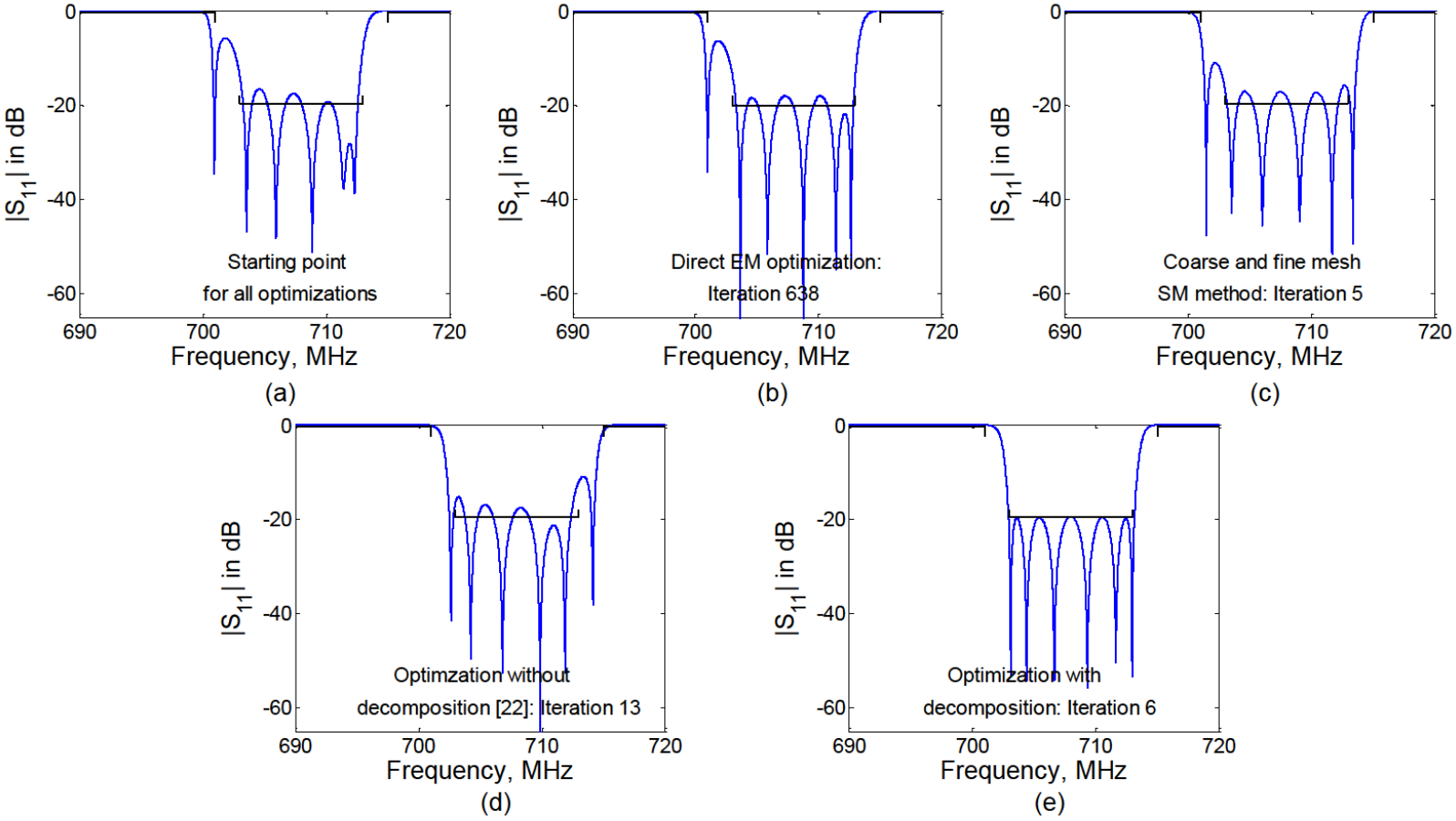
Comparison of Validity Range of the Surrogate Model

Optimization	Optimization method without decomposition	Optimization method with decomposition		
		Sub-optimization 1	Sub-optimization 2	Sub-optimization 3
Design variables	$\boldsymbol{x} = [h_{c1}\ h_{c2}\ h_{c3}\ r_c\ r_p\ w_1\ w_2\ w_3\ w_4\ w_a\ w_b]^T$	$\tilde{\boldsymbol{x}}^{(1)} = [h_{c2}\ h_{c3}\ r_c]^T$	$\tilde{\boldsymbol{x}}^{(2)} = [h_{c1}\ r_p\ w_1\ w_2\ w_a]^T$	$\tilde{\boldsymbol{x}}^{(3)} = [w_3\ w_4\ w_b]^T$
Trust radius (deviation from central point)	**[0.05 0.05 0.025 0.05 0.1 0.1 0.1 0.1 0.1 0.1 0.1]^T**	**[0.5 0.24 0.42]^T**	**[1.1 2.0 2.0 2.0 1.7]^T**	**[1.6 2.0 2.0]^T**
Surrogate model training error	3.56%	3.2274%	3.2278%	3.4281%
Surrogate model test error	4.5247%	3.954%	3.7451%	3.814%

Results of Crossover in the First Iteration



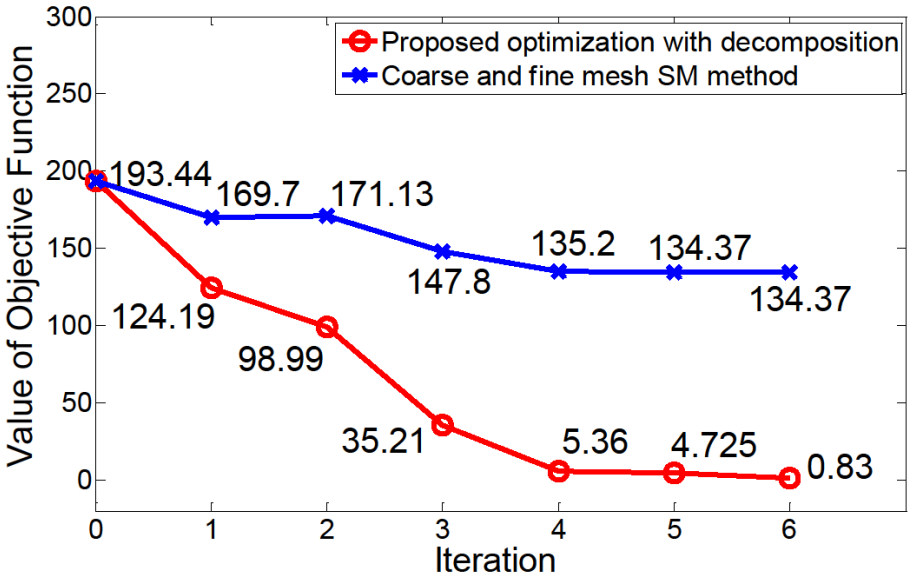
Comparison of Different Optimization Methods

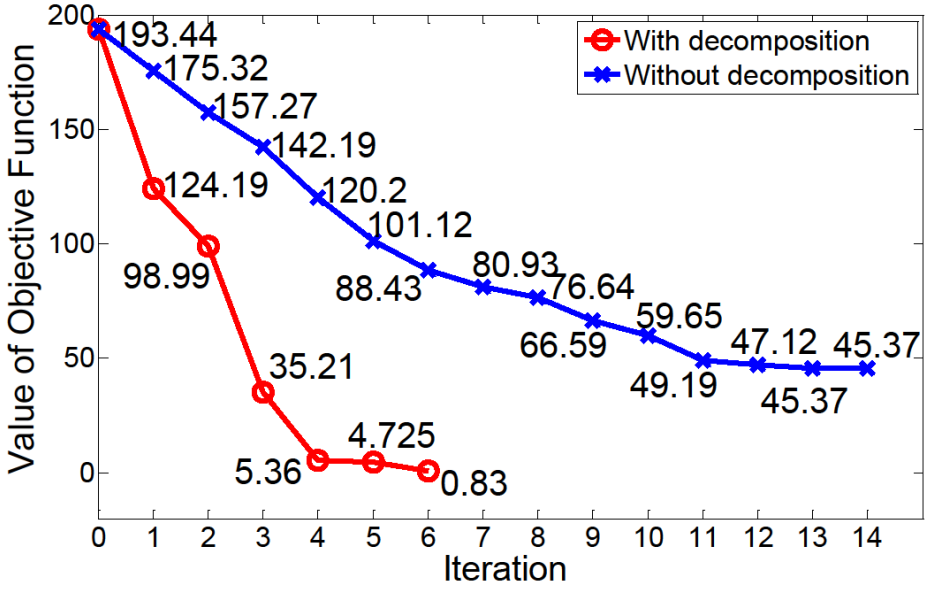


CPU Time Comparison

Optimization	Direct EM optimization	Coarse and fine mesh SM optimization	Opt. Method without decomposition	Proposed optimization with decomposition
Time for derivative calculations	-	-	13m 16s (1^{st} order)	**29m 28s (1^{st} &2^{nd} order)**
Fine model evaluation time per sample	11m 32s	11m 32s	13m 16s	**13m 16s**
No. of fine model evaluations in parallel per iteration	1	1	98	25+25+16
No. of iterations	638	5	13	6
Evaluation time for all fine models	11.5m x 638	11.53m x (5+1)	13.27m x (13+1)	13.27m x 6 + 13.27m x 6
Time for surrogate modeling and optimization	-		3.1m x 13	2m x 6
No. of coarse models	-	1165	-	-
Time for each coarse model evaluation	-	5.083m	-	-
Total time	122.6h	98.69h	309.73m	200.54m

Objective Value Comparison





Contribution-II

- The proposed method decomposes a single large optimization into multiple smaller sub-optimizations to improve optimization efficiency
- Construction of surrogate model and optimization of each sub-problem are performed in parallel.
- Speed up is achieved by using the proposed decomposition method combined with parallel computations.
- Has better chance of avoiding local minima by incorporating crossover mechanism in the optimization process.

Future Directions

- Explore the optimization efficiency for large number of design variables (n>20)
- Higher order regression techniques.
- Use of co-ordinate rotation to reduce the interactions between design variables.
- Yield-driven optimization.
- Use of the proposed parallel approach for active circuit design.

THANK YOU